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Modelling the fate of organic microcontaminants in wastewater treatment and agricultural reuse – Experiences from two existing cases

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1. Theoretical background - Reasons for performing this work and progress beyond the state of the art

In areas characterized by water scarcity, wastewater represents an appealing option for use in agriculture for irrigation purposes. Down-the-drain organic microcontaminants (e.g., pharmaceuticals and personal care products) entering municipal wastewater treatment plants (WWTPs) typically undergo incomplete removal. Hence, irrigation with treated effluents represents a vector of microcontaminants to agricultural systems and may eventually result in the uptake and accumulation in irrigated crops, possibly leading to human exposure via crop consumption. While most of existing evidence on crop uptake following irrigation with wastewater has been obtained under lab-scale conditions, only a limited number of studies (e.g., [1, 2]) focused on field-scale agricultural systems, likely due to major experimental efforts.

In this context, modelling tools integrating fate predictions in wastewater treatment and wastewater-irrigated agricultural systems can be highly beneficial for (i) pre-screening of potentially hazardous chemicals; and (ii) scenario analysis, long-term exposure assessment and decision support. To date, integrated models have been established and tested only for ideal and semi-ideal wastewater treatment reuse scenarios [3], hence lacking a validation for real catchments.

In this study, integrated models of different complexity were used to simulate the fate of excreted organic microcontaminants during transport in sewers, wastewater treatment and uptake in crops irrigated with treated effluent. Integrated models were adapted and tested for two existing scenarios, where direct reuse of treated wastewater for crop irrigation is a long-term (>10 years) established practice.

2. Experimental setup and main methods used in this work

We selected two existing catchments (1 and 2), located in Southern Europe, where wastewater is collected from urban areas (with low industrial contribution), treated in municipal WWTPs and reused for irrigation and cultivation of food crops (e.g., lettuce, corn). Integrated models, adapted to each catchment,

were used to predict the fate of the pharmaceuticals carbamazepine, diclofenac, ibuprofen, ketoprofen and furosemide. Catchment 1 (Spain) was simulated using a steady-state approach by combining the WWTP model Activity SimpleTreat [4] and a recently developed plant uptake model with phloem transport [5]. Catchment 2 (Italy) was simulated using the dynamic IUWS-MP model library [6], which includes sewer network, municipal WWTP and receiving river, and was extended with a dynamic plant uptake model. An overview of the boundaries of the systems is given in Figure 1. Model input included catchment-specific characteristics (e.g., residential population), chemical consumption and excretion (where relevant) and chemical properties (e.g., partitioning coefficients, biodegradation rates). Both models were calibrated and/or validated using measurements for microcontaminants in WWTP influents, effluents and receiving environments. In the case of Catchment 1, the plant uptake model was validated with experimental results from dedicated greenhouse experiments with irrigated lettuce [7].

3. Important findings

In the current abstract, preliminary modelling results are presented for Catchment 1. Calibration of Activity SimpleTreat against measured WWTP concentrations of ibuprofen, ketoprofen and diclofenac resulted in the estimation of biodegradation rate constants (5.02, 0.08 and 0.22 L g⁻¹ d⁻¹, respectively) in line with previous experimental findings. No removal of carbamazepine had been experimentally observed, hence confirming its persistence to biodegradation. Uptake of microcontaminants in lettuce was then simulated and compared with empirical results. Addition of phloem transport was instrumental for describing translocation of weak acids (pK_a < 5), such as diclofenac, that are subject to ion trapping in phloem (pH 8). Model simulations confirmed the uptake and translocation potential of two of the investigated microcontaminants, i.e. carbamazepine and diclofenac. In particular, simulated concentration in lettuce leaves were within 70%-130% of measurements for carbamazepine (Figure 2) and diclofenac, thus indicating comparably good prediction of accumulation in edible crop tissue for these two chemicals.

Future work as part of the current study will include: (i) a comparison between the two modelling approaches (steady-state and dynamic) used for the two catchments; (ii) estimation of human exposure via consumption of irrigated food crops; (iii) scenario simulations to estimate uptake in crops following long-term irrigation reuse.

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4. Figures

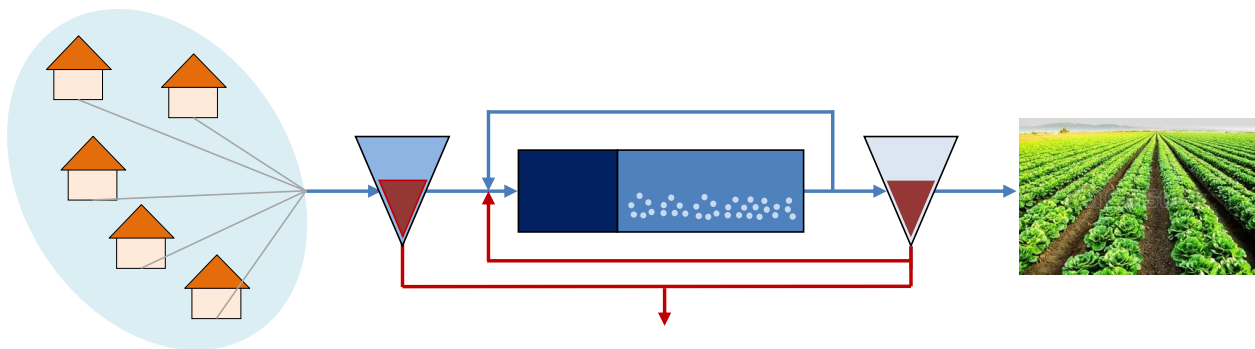


Figure 1. Overview of the wastewater collection, treatment and reuse system in Catchment 1 and 2 and described in integrated models.

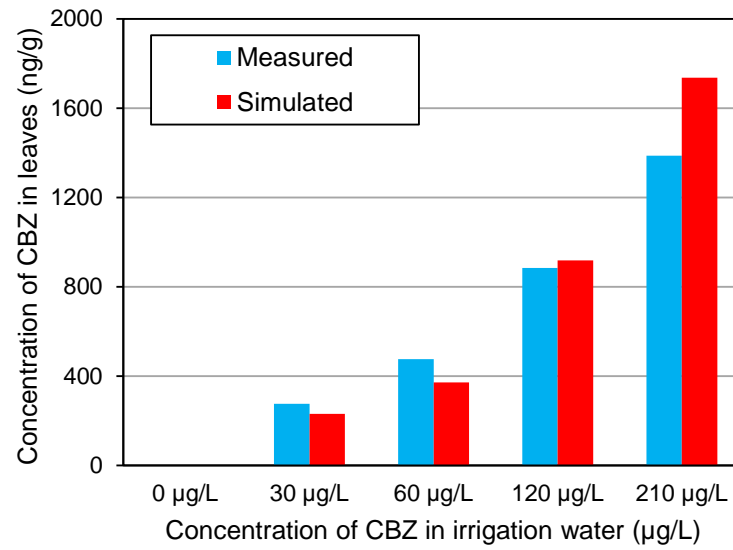


Figure 2. Measurements and simulations of uptaken concentration of carbamazepine (CBZ) in lettuce leaves.